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VERITAS: a high-flux neutron reflectometer with vertical sample geometry for a long pulse spallation source

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Abstract.

An instrument concept of a reflectometer with a vertical sample geometry fitted to the long pulse structure of a spallation source, called “VERITAS” at the ESS, is presented. It focuses on designing a reflectometer with high intensity at the lowest possible background following the users’ demand to investigate thin layers or interfacial areas in the sub-nanometer length scale. The high intensity approach of the vertical reflectometer fits very well to the long pulse structure of the ESS. Its main goal is to deliver as much usable intensity as possible at the sample position and be able to access a reflectivity range of 8 orders of magnitude and more. The concept assures that the reflectivity measurements can be performed in its best way to maximize the flux delivered to the sample. The reflectometer is optimized for studies of (magnetic) layers having thicknesses down to 5 Å and a surface area of 1x1cm². With reflectivity measurements the depth-resolved, laterally averaged chemical and magnetic profile can be investigated. By using polarised neutrons, additional vector information on the in-plane magnetic correlations (off-specular scattering at the µm length scale, GISANS at the nm length scale) can be studied. The full polarisation analysis could be used for soft matter samples to correct for incoherent scattering which is presently limiting neutron reflectivity studies to a reflectivity range on the order of 10⁻⁶.

1. Introduction

The European Spallation Source (ESS) will provide neutron pulses with a width of $\tau=2.84\text{ms}$ and a repetition rate of 14Hz. Though the average flux at the ESS (with its TDR moderator) will be practically equal to the one at the ILL, the time structure of the neutron beam allows for a drastic gain in intensity for time-of-flight instruments due to the 25 times higher peak intensity of the ESS [1]. The



natural resolution of the instrument using the full pulse width is τ/L and defined by the choice of the instrument length L . On the other hand, the artificial narrowing of the pulse width by pulse shaping choppers allows to increase the resolution at the cost of intensity. This opens an exciting opportunity to design a next-generation reflectometer to meet the increasing demand and anticipated scientific challenges. The research topics that will benefit from this reflectometer comprises a wide range of scientific disciplines, ranging from thin film magnetism and novel topological phases in confined geometries, the functionality and properties of hybrid materials in the field of soft and hard matter to the structural biology of membrane proteins. Though the proposed vertical sample geometry excludes the examination of liquid-liquid or liquid-gas interfaces, it nevertheless provides sufficient advantages for soft matter samples that do not require such interfaces and can be measured on the vertical reflectometer with the appropriate sample environment without compromises. Full polarisation analysis will allow measurements of those sample types that were not possible before by making it possible to correct for incoherent background.

The instrument concept presented here, called “VERITAS” the ESS, focuses on designing a reflectometer with high intensity and low background following the high demand of the users to investigate thin layers or interfaces in the sub-nanometer length scale. The high intensity approach of the vertical reflectometer fits very well to the long pulse structure of the ESS. Its main goal is to deliver as much usable intensity as possible to the sample position and be able to access a reflectivity range of 8 orders of magnitude and more.

The concept assures that the reflectivity measurements can be performed in its best way to maximize the flux delivered to the sample. The reflectometer is optimized for studies of (magnetic) layers having thicknesses down to 5\AA and a surface area of $1\times 1\text{cm}^2$. With reflectivity measurements the depth-resolved, laterally averaged chemical and magnetic profile can be investigated. By using polarised neutrons, additional vector information on the in-plane magnetic correlations (off-specular scattering at the μm length scale, GISANS at the nm length scale) can be studied.

The instrument will furthermore be capable to work with a higher wavelength resolution down to 1%. Depending on the operational mode of the instrument, different detector configurations will be used. The detector area will be highly configurable and optimised for the different needs of the specular, off-specular and GISANS-modes.

The design of the vertical reflectometer is based on well-tested components that will be very robust and bear no unpredictable risks for a reliable operation.

1. General philosophy: relaxed Q-resolution machine

The proposed instrument is primarily designed for the investigations of thin interfaces from several nm down to the sub nm range. The main goal is therefore to deliver as much usable intensity as possible at the sample position to be able to access a reflectivity range of 8 orders of magnitude and more. Fig. 1 shows the specular reflectivity curves simulated for a thin Fe-layer for a perfect and relaxed Q-resolutions, respectively. Comparing the two cases it can be noticed that only the minima of the interference pattern are slightly smeared out in the latter case, thus the resolution for the measurement can be drastically relaxed for thin interfacial structures without any loss of information. With a relaxed resolution the neutron intensity on the sample is increased to obtain a detectable signal from an extremely small amount of the scattering material of a thin layer, particularly if it is required to measure the reflectivity up to high Q values.

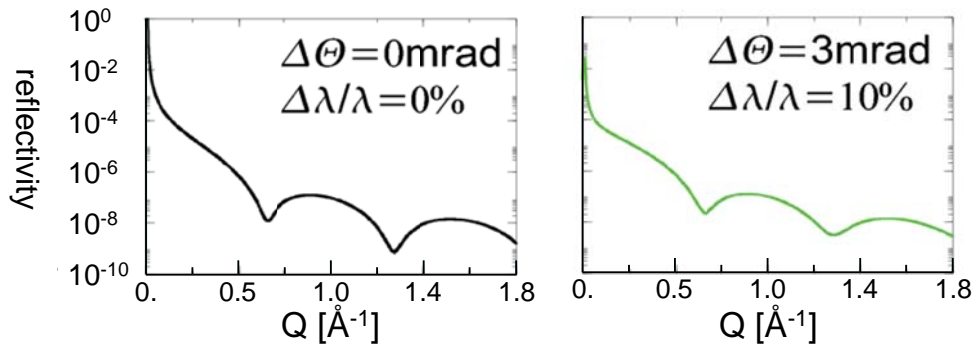


Fig. 1: Simulated reflectivity curve of 10Å thin Fe layer on a Ag substrate for ideal resolution/collimation and for relaxed wavelength resolution/collimation.

The pulse width τ and the instrument length L from the moderator to the detector impose physical limits on the main instrument parameters – the natural λ -resolution and the wavelength band $\Delta\lambda$, are both directly determined by the choice of τ and L :

$$\frac{\Delta\lambda}{\lambda} \propto \frac{\tau}{T} \propto \frac{\tau}{L} \quad \Delta\lambda \propto \frac{1}{L} \quad (1)$$

(T – the time of flight of neutrons from the moderator to the detector). To achieve a resolution of 10% for $\tau=2.86\text{ms}$ at the ESS and to use a maximum of neutrons from the spectrum centered around a wavelength of 3Å, the instrument length L is fixed at about 36m. When L is chosen no further relaxation of the wavelength resolution is possible while the increase in the resolution can be achieved by a shortening of the pulse length. In turn the repetition rate of 14Hz and the choice of instrument length defines the wavelength band of the instrument to $\Delta\lambda=8\text{Å}$.

2. General instrument layout

The general layout of the instrument is depicted in Fig. 2, the schematic diagram of the instrument is shown in Fig. 3. The overall length up to the detector position is 36m allowing a wavelength resolution of 10% (see above) by making use of the full length of the ESS pulse.

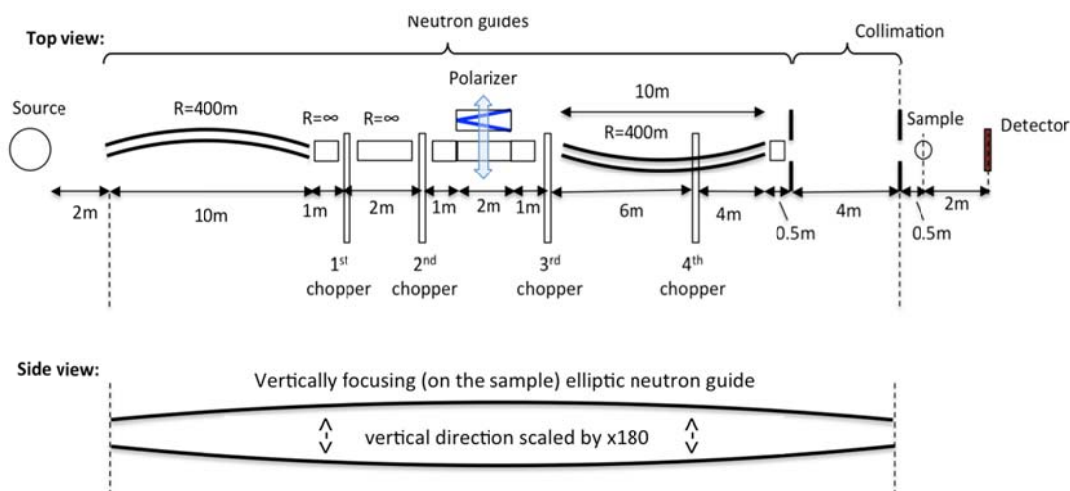


Fig. 2: The top and side view of VERITAS. The moderator is on the left hand side.

2.1. Neutron guide design:

The instrument guide is S-shaped and made of two curved neutron guides ($R=400\text{m}$) with a 7m long straight neutron guide at the inflection point (see Fig. 2). The use of the S-shaped neutron guide prevents the direct line-of-sight of the primary and secondary radiation sources. The movable parts (choppers, polariser changer, etc.) are positioned downstream of the neutron beam beyond the biological shielding and thus can be freely accessed during the operation of the ESS. The basic guide parameters are listed in Table 1. The neutron guide width of 30mm is chosen to allow the complete filling of the phase space of the guide for a moderator width of 10cm. To increase the incident neutron intensity for reflectivity measurements on small samples, the incident neutron beam is focused along the vertical direction onto the sample using a focusing elliptical neutron guide. A comparison of the intensities at the sample position (for a sample size of $1 \times 1 \text{ cm}^2$) of such a setup to a straight guide with a cross section of $3 \times 12 \text{ cm}^2$ and mirrors with $m=2$ coating shows a clear increase in the beam intensity by at least a factor of 4 for the elliptical focusing option (see Fig. 3).

An elliptical guide (see Table 1 for the shape) with the same length and $m=3$ coating for the last 4m will be used.

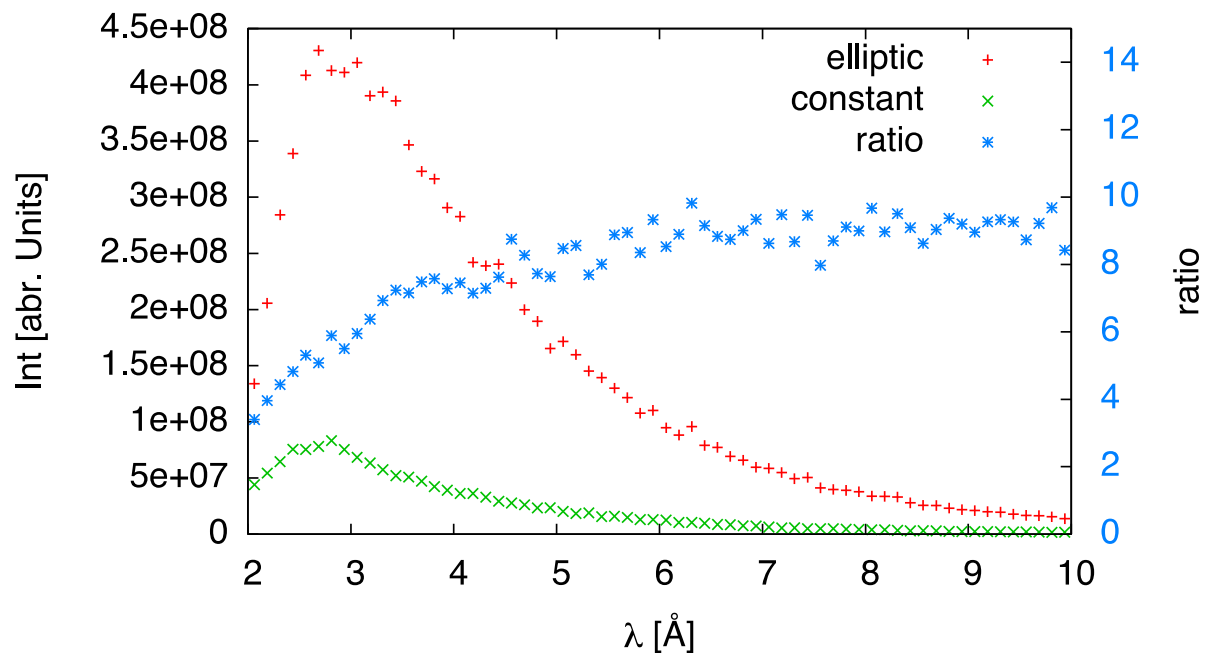


Fig. 3: Comparison of the intensity at the sample position with a sample size of $1 \times 1 \text{ cm}^2$ for elliptical and constant cross section neutron guides.

2.2. Chopper design:

The time-distance diagram for the low resolution mode is shown in Fig. 4a. The first chopper at 13m is the band selection chopper selecting an 8 Å broad wavelength band. The band from 2 to 10 Å will provide the highest intensity. The wavelength band can be selected arbitrarily in a range between 2 and 32 Å . This is important in the case one wants to adjust the reciprocal space to a specific scientific question, e.g. separating the off-specular scattering signal from the direct beam or in the GISANS mode for separating reflections from each other. The additional choppers ((2) at 15m, (3) at 19m and

(4) at 25m) serve as frame overlap choppers to prevent contaminations of very high wavelength neutrons of more than 50\AA .

	gth				Exit height	Exit width	ng		Coating left	Coating right
1	10.0m	+400m	95.8mm	30mm	194.5mm	30mm	m=3.0	m=3.0	m=3	m=4
2	1.0m	∞	194.5mm	30mm	198.5mm	30mm	m=3.0	m=3.0	m=3	m=3
3	2.0m	∞	198.5mm	30mm	202.7mm	30mm	m=3.0	m=3.0	m=3	m=3
4	4.0m	∞	202.7mm	30mm	202.5mm	30mm	m=3.0	m=3.0	m=3	m=3
5	6.0m	-400m	202.5mm	30mm	180.5mm	30mm	m=3.0	m=3.0	m=4	m=3
6	4.0m	-400m	180.5mm	30mm	145.5mm	30mm	m=3.0	m=3.0	m=4	m=3
7	0.5m	∞	145.5mm	30mm	140.0mm	30mm	m=3.0	m=3.0	m=3	m=3
8	4.0m	∞	140.0mm	30mm	54.0mm	30mm	m=3.0	m=3.0	absorber	absorber

Table 1: Basic guide design parameters. To avoid the depolarization of the neutron beam, all guides after the polarizing cavity (from section 4) are coated with non-magnetic supermirrors. Geometric parameters of the elliptic guide were selected to maximize the brilliance transfer, while keeping the guide's cross-section reasonably small for a practical chopper design.

In order to achieve a high wavelength resolution for the proposed design, the natural pulse width has to be reduced according to Eq. (1). Technically the sub-pulse duration will be defined by a pulse-shaping chopper installed at 13m from the source. Each sub-pulse will provide neutrons arriving at the detector during a certain time interval (time sub-frame) and covering a certain wavelength band (wavelength sub-frame), see Fig. 4b. For the optimal use of all neutrons from the long ESS pulse, a sequence of sub-pulses will be selected that the wavelength band of subsequent sub-frames will overlap. Then the available wavelength band from 2 to 10\AA will be completely covered thus avoiding gaps in Q. It is necessary, however, that the time sub-frames of these sub-pulses are well separated to avoid ambiguity in the wavelength (i.e. in Q) determination. The high-resolution choppers will be installed just behind Ch.1 and Ch.3 (see Fig. 4b).

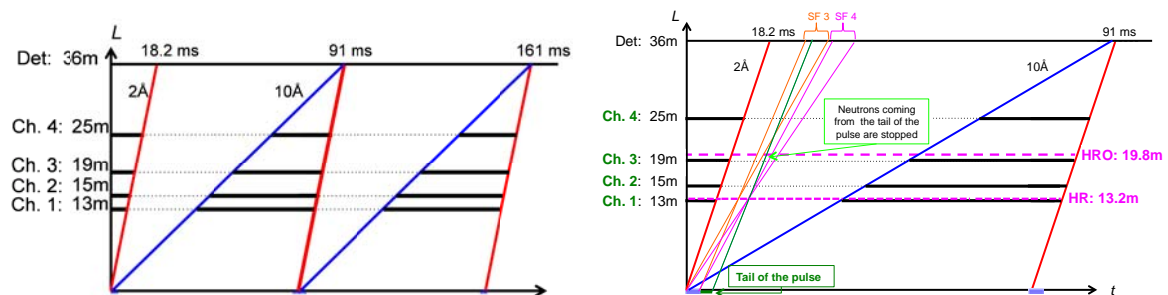


Fig. 4: Time-distance diagrams of the (a) low and (b) high resolution mode

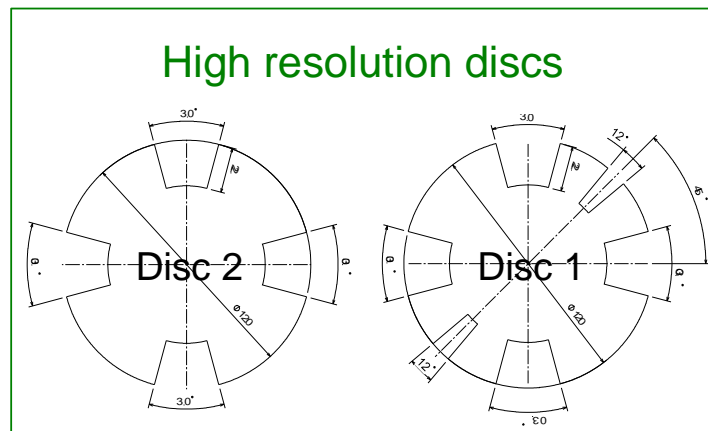


Fig. 5: A double disc chopper allowing different openings by setting an offset angle between the discs.

Different resolutions require a variable opening of the pulse-shaping high-resolution chopper. Therefore we use a double disc chopper (see Fig. 5) that will allow different openings by setting an offset angle between the discs. For a 1% wavelength resolution mode, an offset angle of 45° will result in two openings of 10° . In the 3% and 5% modes, the offset angles will be set between -12.5° and $+12.5^\circ$, leading to 4 windows and a variable opening from $0-25^\circ$. The frequency of the sub-pulses has to be an integer multiple of the frequency of the ESS source, otherwise the timing of the sub-pulses will continuously shift relative to the ESS pulses. The simulated time and wavelength intensity distributions for the 1, 3 and 5% resolution modes show a clear separation of the time sub-frames and an overlap of the wavelength sub-frames (see Fig. 6). It is important to note that in all three modes, the $\Delta\lambda/\lambda$ value is not constant because the pulse length, whether directly from the ESS or from the HM-chopper, is always constant, while the λ values change.

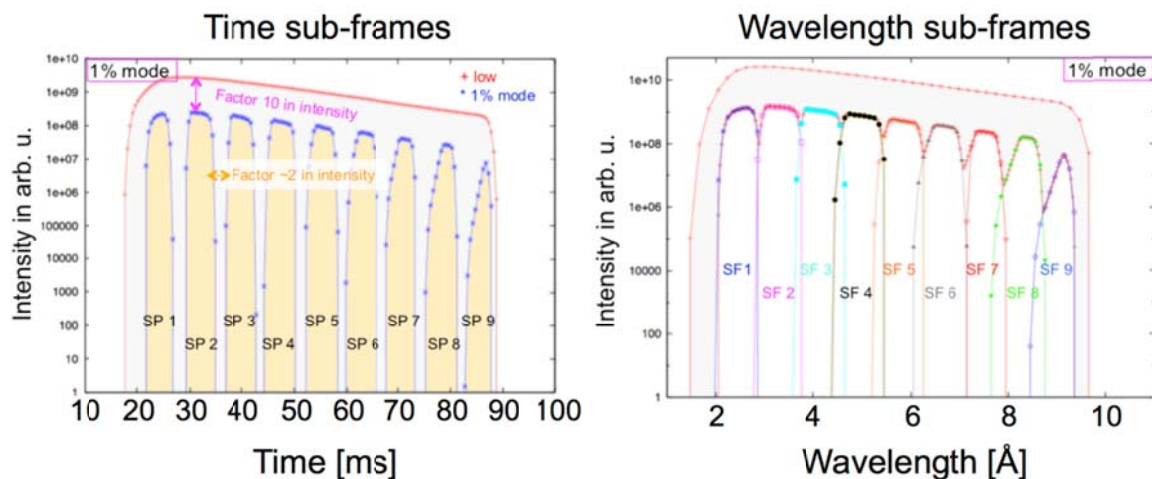


Fig. 6: The simulated time and wavelength intensity distributions for the 1% wavelength resolution modes. The low wavelength resolution curves ($\Delta\lambda/\lambda=10\%$) are shown as envelopes.

2.3. Polarization option:

In the polarized mode, the central 2m long piece of the guide (see Fig.2) will be replaced by another one equipped with a polarizing cavity which is built upon thin, 0.3mm thick, Si wafers coated with $m=5$ Fe/Si supermirrors working in transmission [2]. This solution leads to high values of neutron beam polarization (see Fig. 7) with small intensity losses over the whole wavelength band and allows practically for instant-switch between polarizing and non-polarizing operation modes without affecting the overall beam propagation. Even higher polarization of the neutron beam of more than 99% can be achieved using an optional ^3He neutron spin filter with a wide band neutron adiabatic RF-flipper, resulting in a drop of the beam intensity of about 25%. It should be noted that all sections after the polarizer will be coated by non-magnetic supermirrors.

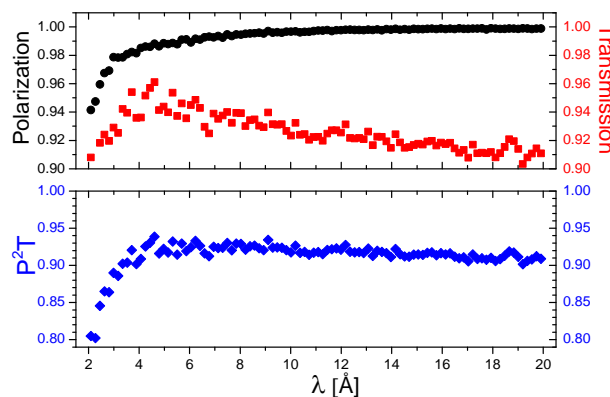


Fig. 7: Polarization P , transmission T of the selected spin component and the figure of merit P^2T of the polarizing cavity setup.

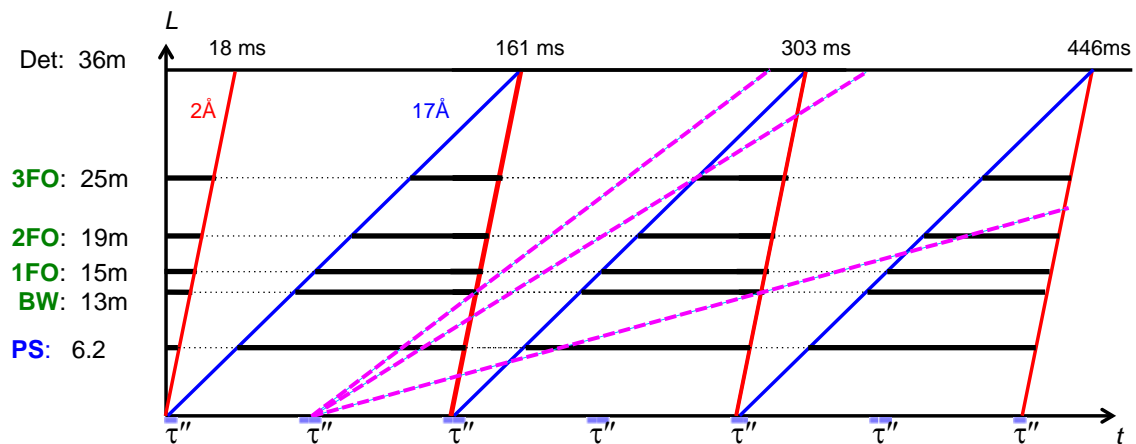


Fig. 8: Time-distance diagram for the kinetic mode of the 1 pulse skipping mode (7Hz), i.e. skipping every second pulse of the ESS source.

2.4. Kinetic mode:

For kinetic measurements it is desirable to cover a large Q -range for a single angular setting to allow measuring of the kinetic processes on time scales of one second and less. The design of VERITAS enables one to extend the Q range beyond the ratio of $Q_{\text{max}}/Q_{\text{min}} \approx 5$ in the basic chopper mode by

skipping one or more pulses. This can be easily realized by placing one additional chopper (PS) at 6.2m distance from the source blocking the neutrons coming from the second (7Hz mode), third (4.7Hz) or fourth (3.5Hz) pulse as depicted in the time-distance diagram in Fig. 8 for the 1 pulse skipping mode. The corresponding choppers' settings are listed in Table 2, and e.g. the 3 pulse skipping mode enables one to measure a complete reflectivity curve in a Q range from 0.0075\AA^{-1} (total reflectivity plateau) up to 0.12\AA^{-1} ($\sim 10^{-5}$ level depending on the sample) in one shot with a time resolution of 286ms as shown in Figure 9.

Mode	PS[°]	BW[°]	1FO[°]	2FO[°]	3FO[°]	f[Hz]	Time[ms]	Q-ratio
1 pulse	-66.2	-84.9	97.1	121.1	156.4	7	143	9
2 pulse	-40.9	-79.0	-90.3	-112.6	-145.3	4.7	212	12
3 pulse	-39.4	-76.0	-86.9	-108.3	-139.7	3.5	286	16

Table 2. The different parameters of the chopper settings used in the pulse skipping mode.

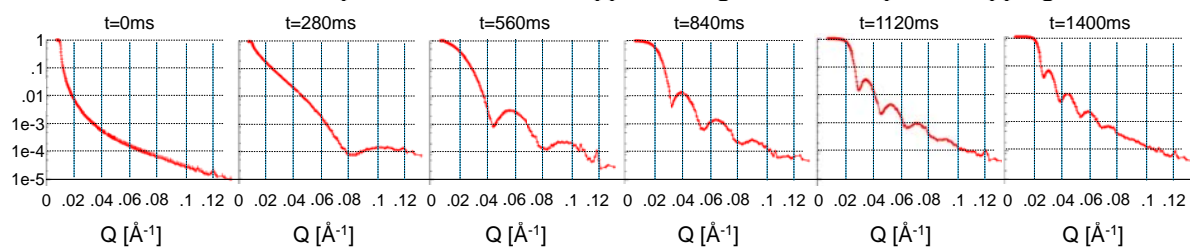


Fig. 9: Simulation of the reflectivity of a Ni thin film on a Si substrate growing in-situ with a growth rate of $28.5\text{\AA}/\text{s}$ inside an MBE and recorded in a time interval of 280 ms on a 1cm^2 sample. The parameters are taken for the low resolution mode in the 3 pulse skipping mode.

3. Performance of the setup.

Taking the basic setup, the intensity-wavelength distribution is simulated for the proposed 10% wavelength resolution (see Fig. 10). The intensity scale is shown for a measurement time of one second and a beam collimation of 3mrad (2mrad Gaussian equivalent) at a spot size of 1cm^2 . The integrated intensity over the full wavelength range amounts to $2.4 \times 10^8 \text{ n/cm}^2$ for each single pulse of the ESS. For the integrated intensity per second this value has to be multiplied by the repetition rate of the ESS (14Hz) leading to $3.4 \times 10^9 \text{ n/cm}^2/\text{s}$ (see Fig. 10). The horizontal divergence profile is depicted in the inset of Fig. 10 showing a smooth distribution and demonstrating that the setup accepts the full divergence of the beam through the collimation. The slight wiggles in the profile are due to the polygonal structure used for the simulation of the curved guide. They will disappear by the use of continuously curved sections at the real instrument. In the GISANS mode the vertical focusing is disabled for a perfect collimation based on a fixed collimation length of 4m. The resolution can be adapted to the needed values in the vertical and horizontal direction. Fig. 11 shows the resulting intensity and the vertical divergence distribution (inset) at the sample position. A total flux of $1.0 \times 10^8 \text{ n/cm}^2/\text{s}$ at 3mrad collimation (2mrad in Gaussian approximation) in both direction is available with a clean vertical divergence profile. The integrated intensity over the full wavelength band will amount to $1.0 \cdot 10^8 \text{ n/cm}^2/\text{s}$.

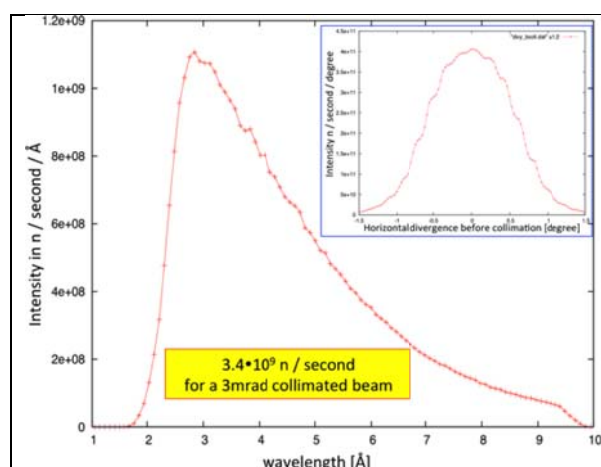


Fig. 10: Spectrum and divergence profile for the low resolution setup of the reflectometer in the lowest wavelength band from 2-10 Å and a beam collimation of 3 mrad (Boxcar). The inset shows the horizontal divergence profile in front of the collimation.

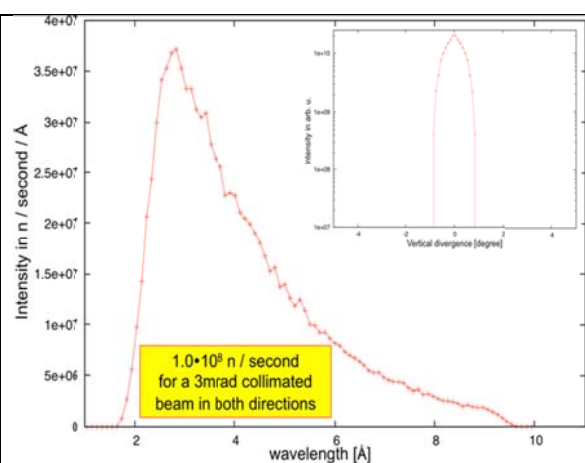


Fig. 11: Spectrum and divergence profile for the GISANS setup in the low resolution setup of the reflectometer in the lowest wavelength band from 2-10 Å and a beam collimation of 3 mrad (Boxcar). The inset shows the vertical divergence profile.

The suggested reflectometer will provide an extremely high flux, exceeding the flux which is currently achievable at the best reflectometers in the world. A 25 times gain is expected in comparison with D17 at the ILL [3]. The simulations above are supported by simple estimations: (i) the average flux at the ILL and ESS is about equal, the chopping of the beam will result in the losses of the useful neutron intensity because of the blocking of the neutron beam between the neutron pulses produced by the choppers; (ii) the opening time is defined by the ratio of the pulse width to their period that is approximately equal to 1/25; (iii) such pulse structure is naturally produced by the ESS, thus no losses related to the time structuring of the neutron beam will occur. Therefore, assuming that other beam parameters are similar, the expected gain is about 25.

4. Conclusions

The instrument concept presented above allows to design a very flexible vertical sample reflectometer for specular reflectivity and off-specular scattering as well GISANS investigations (in the pinhole geometry) at a modern long pulse source. An elliptically focusing neutron guide gives a gain of a factor 4 in intensity compared to a straight guide.

As the length of the instrument depends on the pulse structure of the source and the resolution of the instrument, VERITAS is designed for the ESS, delivering a maximum flux centered around 3 Å with 10% wavelength resolution. It results in a stunning flux of 3.4×10^9 n/cm²/sec at the sample position for a 3 mrad collimated beam (scattering plane) that is 25 times higher than one can achieve with an equivalent instrument at the ILL (e.g. D17). The wavelength resolution can be increased to e.g. 1%, 3% or 5% by using pulse-shaping choppers. Besides the reflectometry mode, VERITAS can be switched into the GISANS mode in seconds, preserving the gain of 25 over an equivalent instrument at the ILL. The huge neutron flux available at the sample position enables one to investigate systems where the sensitivity to a small amount of material or the resolution of small length scales around interfaces in thin film materials is required, something that is not feasible today.

The reflectometry mode as well as the GISANS mode can be further easily combined with a polarizer/analyzer system as well as with the kinetic mode of VERITAS. The need for the polarizer and analyzer system follow the increasing demand in the research field of magnetic nanoparticles (e.g.

assembled in thin films), magnetism, ferroelectricity and superconductivity at interfaces or novel topologically protected magnetic states (e.g. skyrmions) besides many other topics. In addition the polarizer/analyzer system can be used to measure precisely the incoherent background of soft matter samples, increasing the dynamic range of reflectivity and GISANS studies in this science area.

The VERITAS concept at the ESS (or adapted to any other long pulse source with similar strength or even steady reactors like PIK at the PNPI, Russia) allows one to push the limits in thin film science in all directions, making a huge step forward in the instrumentation, particularly for exploiting the full potential of the new spallation sources supporting the users in performing cutting edge science.

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